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ASCR at Los Alamos National Laboratory

Stephen R. Lee
Computer, Computational, and Statistical Sciences Division Leader

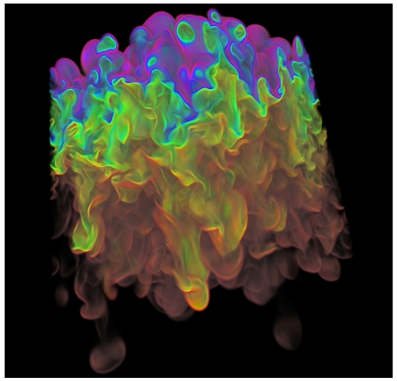
2/2/2016

Outline

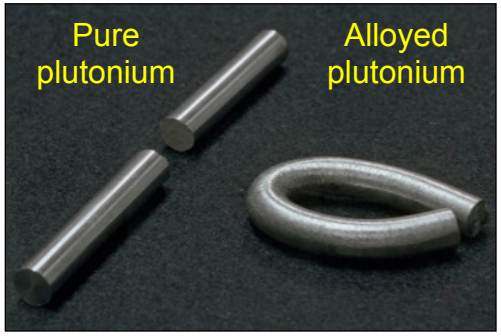
- Laboratory overview
- ASCR at Los Alamos
- CCS – ASCR's computing and math division at Los Alamos
- Facilities: MaRIE
- Computing Strategy
- Los Alamos priorities for ASCR long range planning

As a Laboratory, Los Alamos stewards broad & deep STE capabilities for national security missions

Stockpile Stewardship

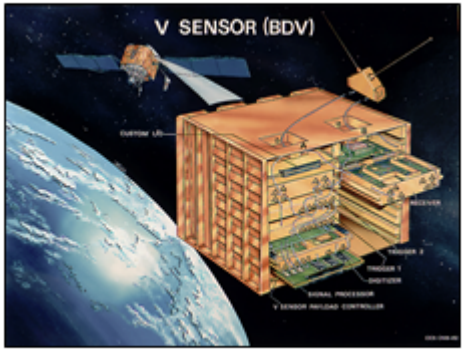


Hydrodynamics:
Turbulence

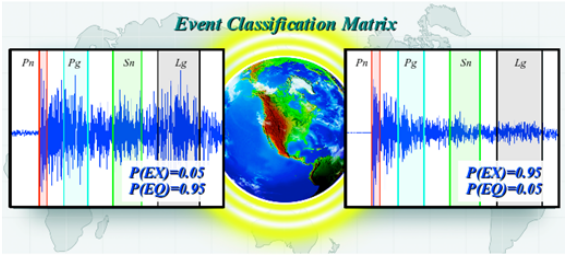


Plutonium Science:
Metallurgy

Global Security

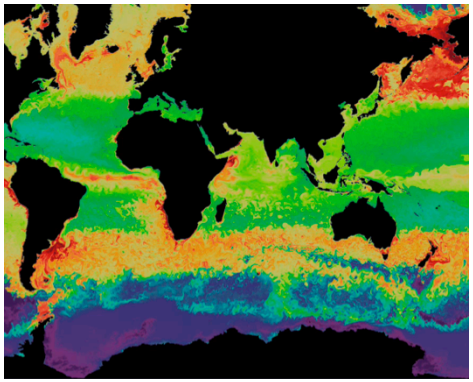


Sensors:
Nuclear detonation verification and treaty monitoring

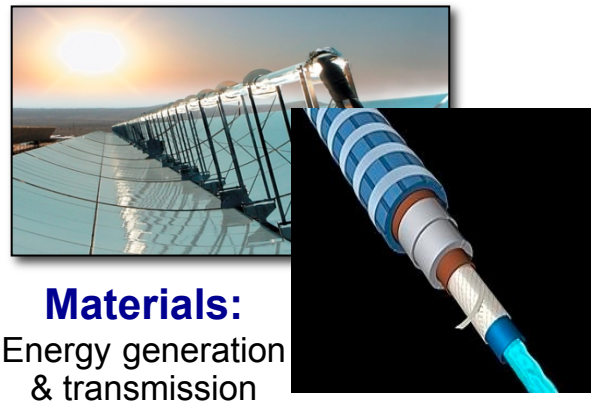


Seismic Detection of Nuclear Explosions

Energy Security



Climate/Energy Impacts:
Measurement, simulation, prediction



Materials:
Energy generation & transmission

Los Alamos NATIONAL LABORATORY EST. 1943

Our Vision, Mission, Values, Goals

Vision

Delivering Science and Technology to protect our nation and promote world stability.

Mission

To solve national security challenges through scientific excellence.

Our Values

We value our people and the extraordinary talents brought to Los Alamos to accomplish our mission. Our values demonstrate this point and communicate the essence of the Laboratory.

- **Service:** Serving our country, our partners, our community, and each other.
- **Excellence:** Ensuring timely mission execution through scientific, operational, and business excellence.
- **Integrity:** Building trust through intellectual honesty, ethical conduct, and individual responsibility.
- **Teamwork:** Collaborating with colleagues and partners, respecting diverse opinions and backgrounds, vigorously debating alternatives, and coming together to achieve the best solutions.
- **Stewardship:** Being good stewards of the taxpayers' dollars, the Laboratory, our community, and the environment
- **Safety and Security:** Ensuring that safety and security are integral to everything we do.

Our Goals

Deliver **national nuclear security** and **broader global security** mission solutions, and

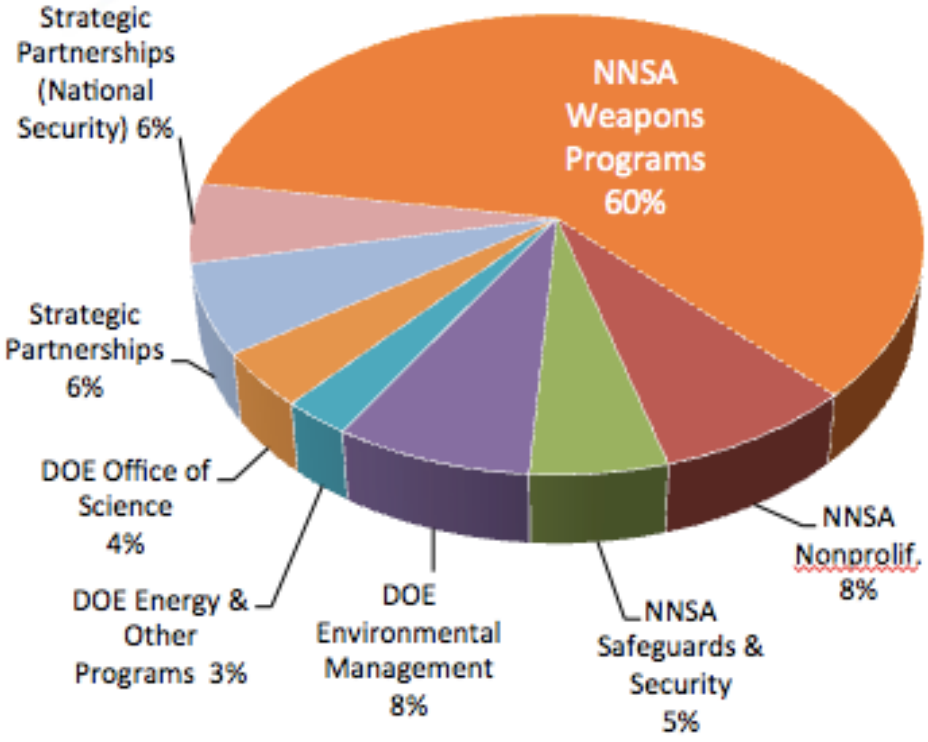
Foster **excellence in science and engineering** disciplines essential for national security missions, *by*

Attracting, inspiring, and developing world-class talent to ensure a vital future workforce, and

Enabling mission delivery through **next-generation facilities, infrastructure, and operational excellence.**

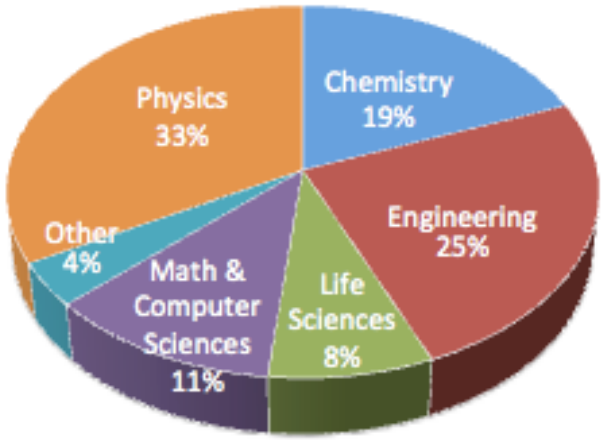
Los Alamos is large and diverse

FY15 Budget Authority: $2.2B



Current Workforce ~ 10,000

Research & Development Disciplines
(21% of workforce)



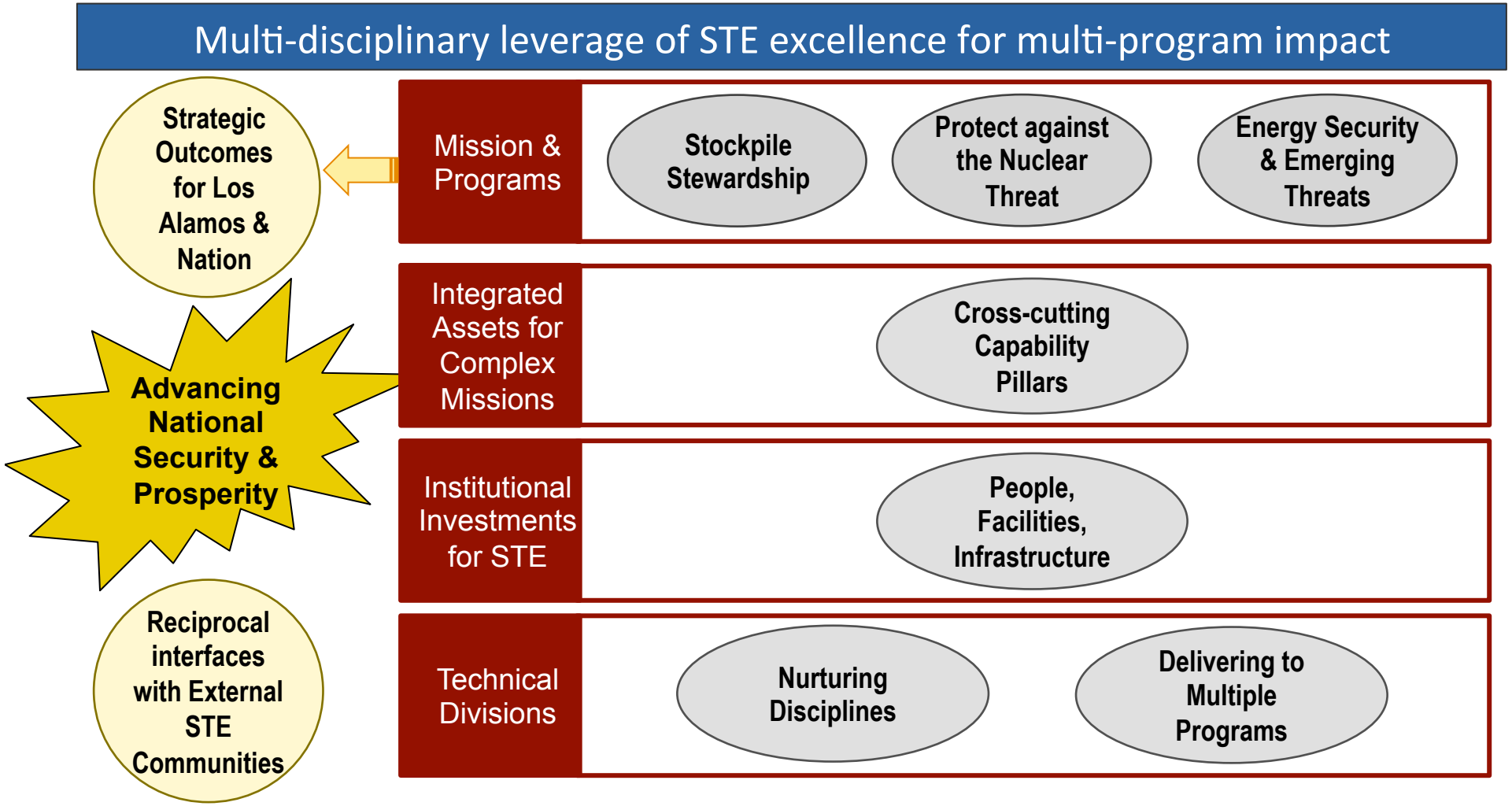
Included in R&D Staff:

~ 350 Postdocs

~ 1,400 Students

Los Alamos is organized to accomplish mission

STE is organized to maximize Los Alamos' value as a National Security Laboratory



At LANL, "capability pillars" build cross-disciplinary teaming expertise for current and future missions

SCIENTIFIC EXCELLENCE FOR NATIONAL SECURITY

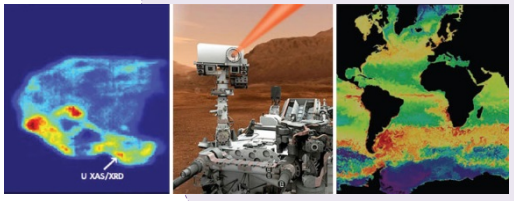
LANL MISSIONS

- Nuclear Deterrence
- Global Security
- Energy & Emerging Threats

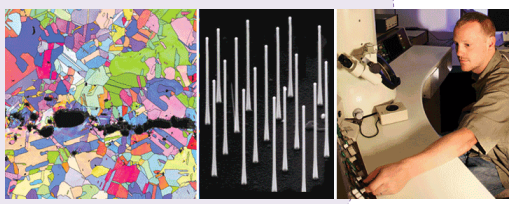
Integrating Assets for Program Execution

CAPABILITY PILLARS

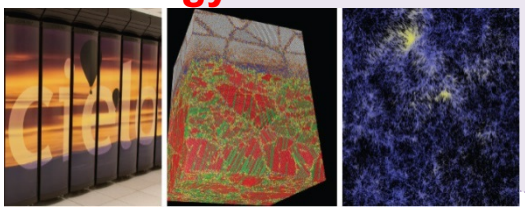
Science of Signatures



Materials for the Future



Information, Science, and Technology for Prediction



Nuclear and Particle Futures

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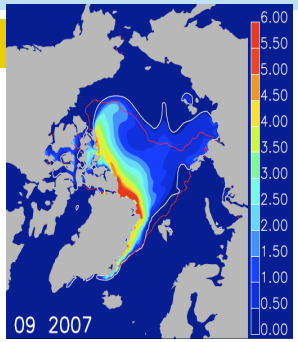
Why does LANL perform DOE Office of Science work?

- Exercise capability through long-term fundamental science;
- Conduct high-risk/high-payoff efforts that enable discoveries and tools that transform understanding of energy and matter and advance national, economic, and energy security;
- Attract, retain, and develop an inventive and innovative workforce connected closely with the best researchers and facilities in the world; and
- Validate quality, relevance, and performance of our work through rigorous standards of competition, peer review, and project management

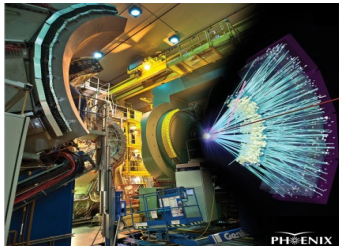
Center for Integrated Nanotechnologies National User Facility

ExMatEx

Exascale Computing Co-design Center



Climate Modeling



RHIC PHENIX Detector

Condensed Matter Physics at 100 T

Medical & R+D Isotope Production

HAWC Gamma-Ray Observatory

W7-X Stellarator at the Max Planck Inst. (FES)

Trinity/NERSC-8 Collaboration

Sandia National Laboratories | NERSC | Los Alamos National Laboratory

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LANL ASCR program organization

ASCR

Rej (Science Programs)

Sarrao (ADTSC)

Computer Science

Pat McCormick

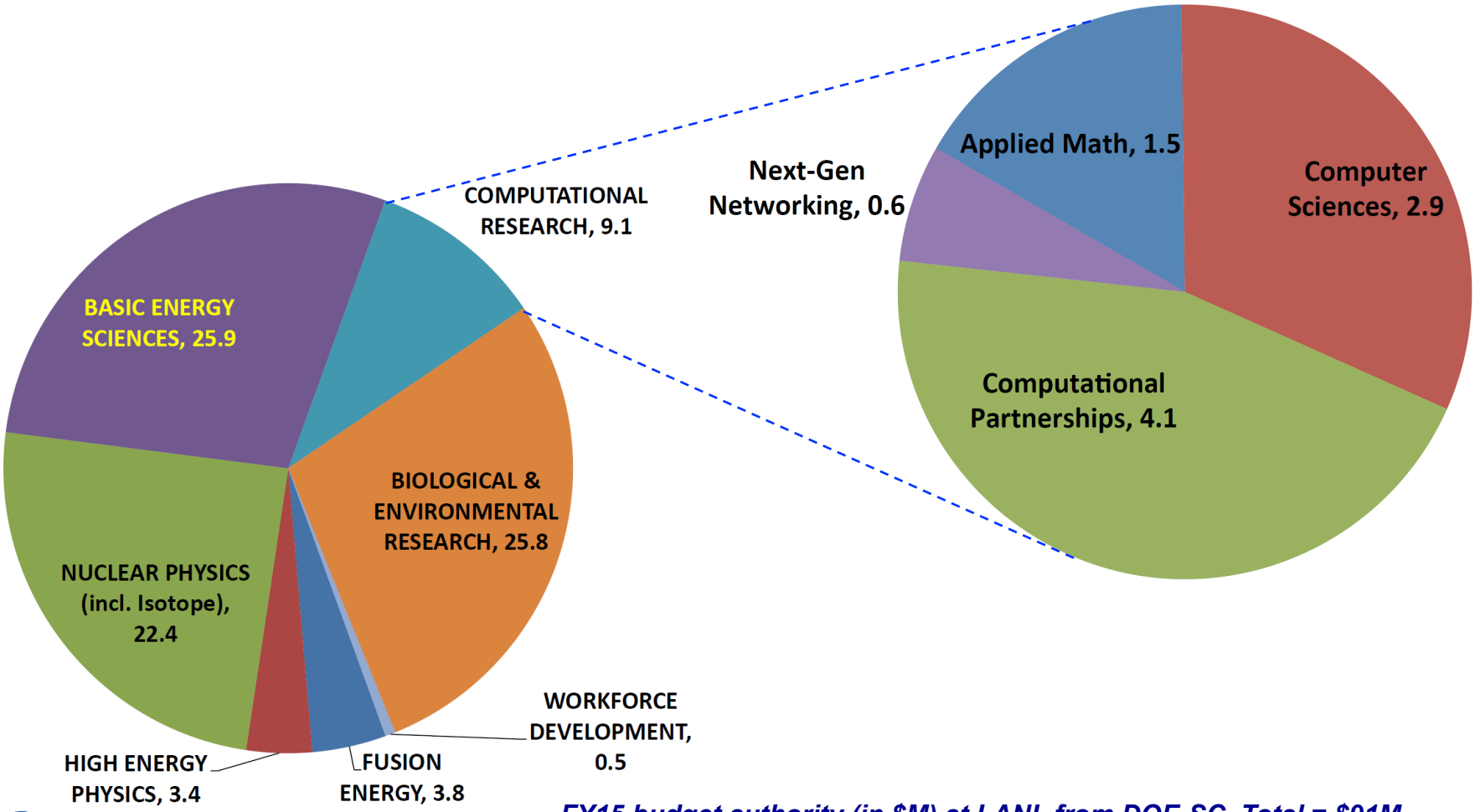
Applied Math

Pieter Swart

Partnerships

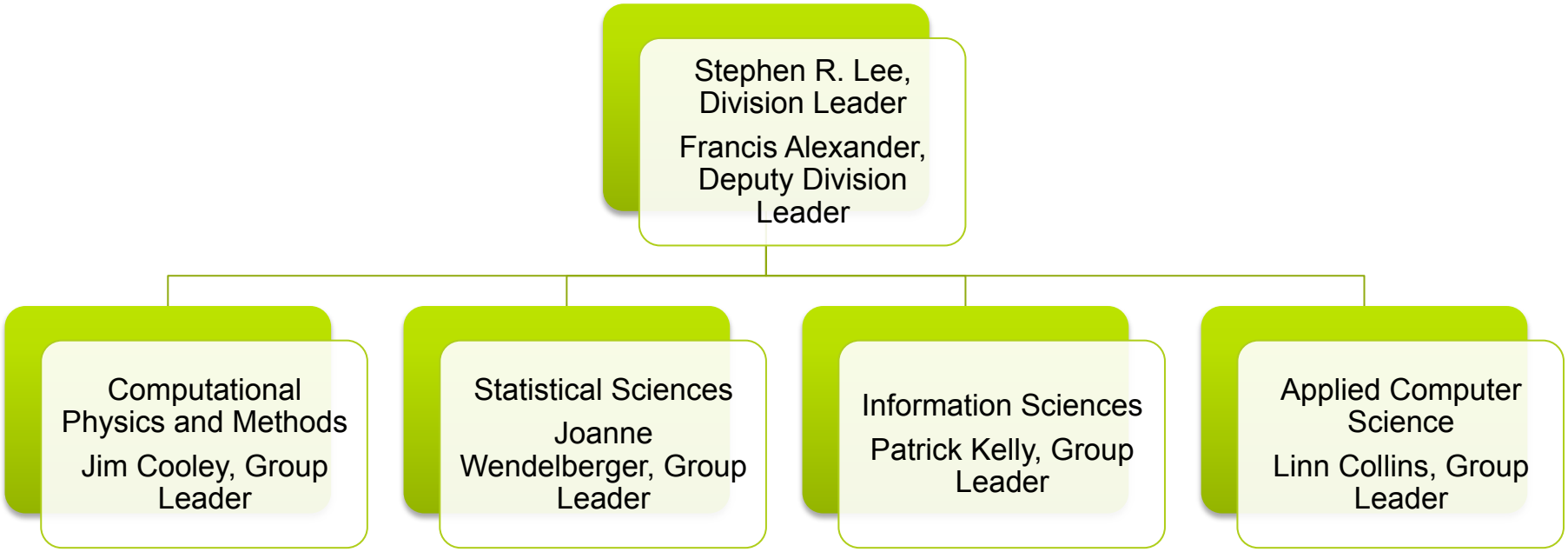
Galen Shipman

ASCR programs were 10% of the LANL Office of Science portfolio in FY15



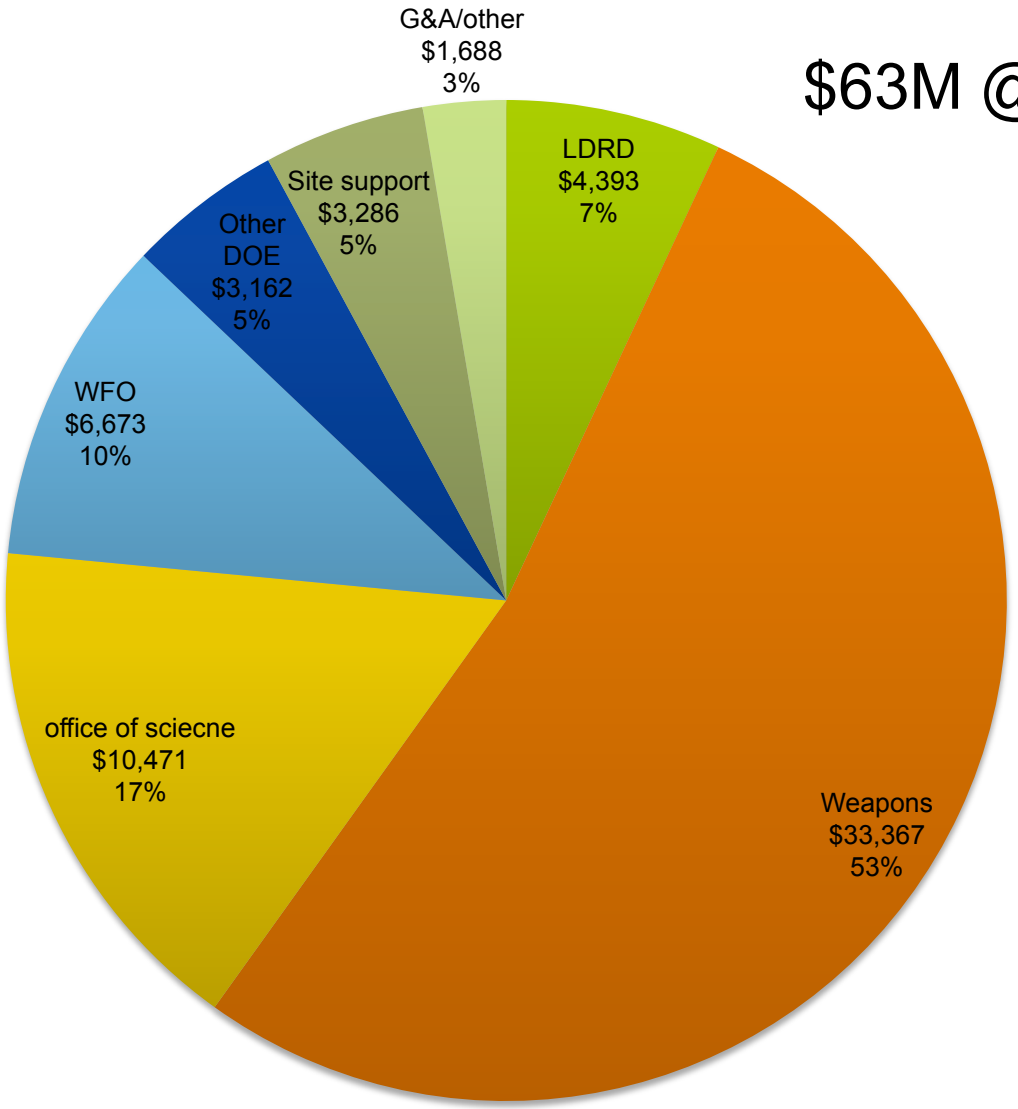
FY15 budget authority (in $M) at LANL from DOE-SC. Total = $91M, including $9.1M from ASCR. Numbers do not include additional $3M from integrated contracts between National Labs, mostly from BER.

The Computer, Computational, and Statistical Sciences Division executes many ASCR programs



150 scientific staff
88% PhD
21 postdocs
~$63M total budget
(CCS does not house the computing center)

CCS Division's budget reflects a healthy mix of mission and science programs



$63M @FY15 close

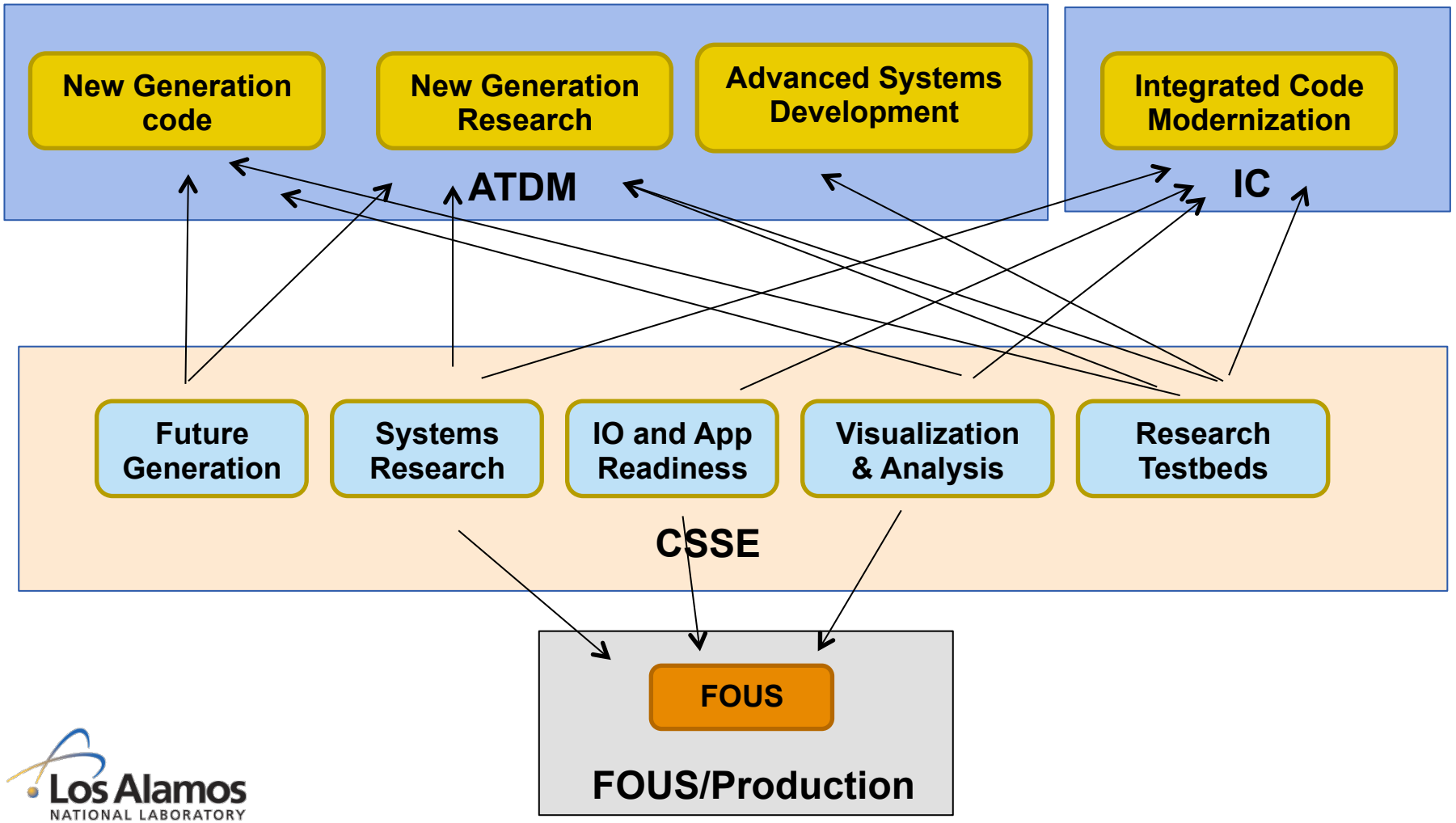
LANL's ASCR portfolio both enables and is enabled by our IS&T Pillar

- **Computational Partnerships: Exascale Co-Design Centers**
  - ExMatEx, ExaCT, CESAR
- **Computational Partnerships: SciDAC**
  - Ahrens - SDAV (Scalable Data Management, Analysis, and Visualization) Institute
  - Gattiker - QUEST Center: Uncertainty Quantification
  - Tang - Plasma Surface Interactions (FES)
  - Price – Predicting Ice Sheet and Climate Evolution at Extreme Scales (BER)
  - Ahrens - Computation-Driven Discovery for Dark Universe (HEP)
  - Carlson - Nuclear Computational Low Energy Initiative (NP)
  - Ringler - Multiscale Methods for Accurate, Efficient, Scale Aware Models of Earth System (BER)
- **Applied Math and Computational Science Projects**
  - Shashkov: Mimetic Methods for Partial Differential Equations
  - Chacon: Enabling Predictive Extended MHD Simulations by the Development of Stable, Accurate, and Scalable Computational Formulations and Solution Methods
  - Chacon: Optimization-based Checkpointing for Hard-fault Recovery in Particle-based Exascale Algorithms
  - DiaMonD: An Integrated Multifaceted Approach to Mathematics at the Interfaces of Data, Models, and Decisions - PIs: Ghattas (UT Austin), Willcox (MIT) (LANL-PI: Vesselinov)
  - Swart - Applied Math Post-doc Program

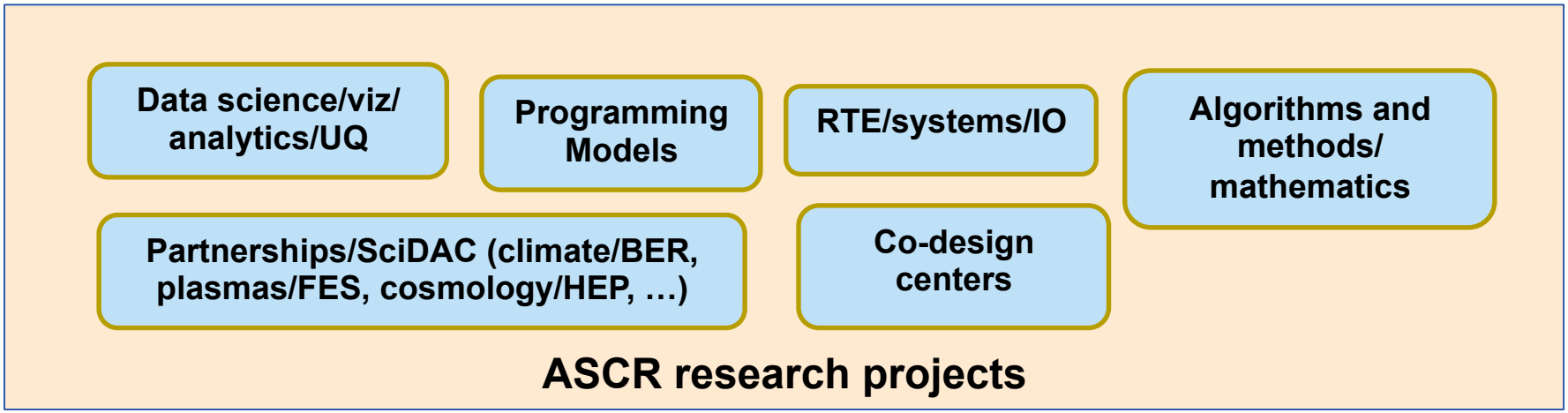
LANL's ASCR portfolio both enables and is enabled by our IS&T Pillar

- **Computer Science Projects**
  - Ahrens: Exploration of Exascale In Situ Data Analysis and Visualization on Emerging Architectures
  - Ahrens: Optimizing the Energy Usage & Cognitive Value of Extreme Scale Data Analysis
  - McCormick: DSLs for In Situ Data Analysis and Visualization on Emerging Architectures
  - McCormick: Abstract Representations for the Extreme-Scale Stack
  - McCormick: A Unified Data Driven Approach for Programming in Situ Analysis
  - Lang: OS and Runtime Support for Application Composition (w/ Sandia)
  - Lang: Unified Memory and Storage Space
  - Lang: Software Defined Networking for HPC Interconnects and its Extension Across Domains
  - Pakin: Whole Program Vectorization
  - Settlemyer: Software Defined Networks for Science Flows (w/ ORNL)
  - Sewel: XVis: Visualization for the Extreme-Scale Scientific-Computation Ecosystem (w/ SNL)
  - Shipman: A Software Defined Storage Approach to Exascale Storage Services (w/ ANL)
  - Woodring: Extreme-Scale Distribution-Based Data Analysis (w/ ANL)
- **Extreme-Scale Productivity**
  - Moulton: BER-lead of Interoperable Design of Extreme-scale Application Software (IDEAS) with ASCR-leads Heroux (SNL) and McInnes (ANL).

ASC CSSE provides mission-centric computer science research for platforms and codes



ASCR provides a crucial research portfolio at LANL that advances science and underpins some ASC developments



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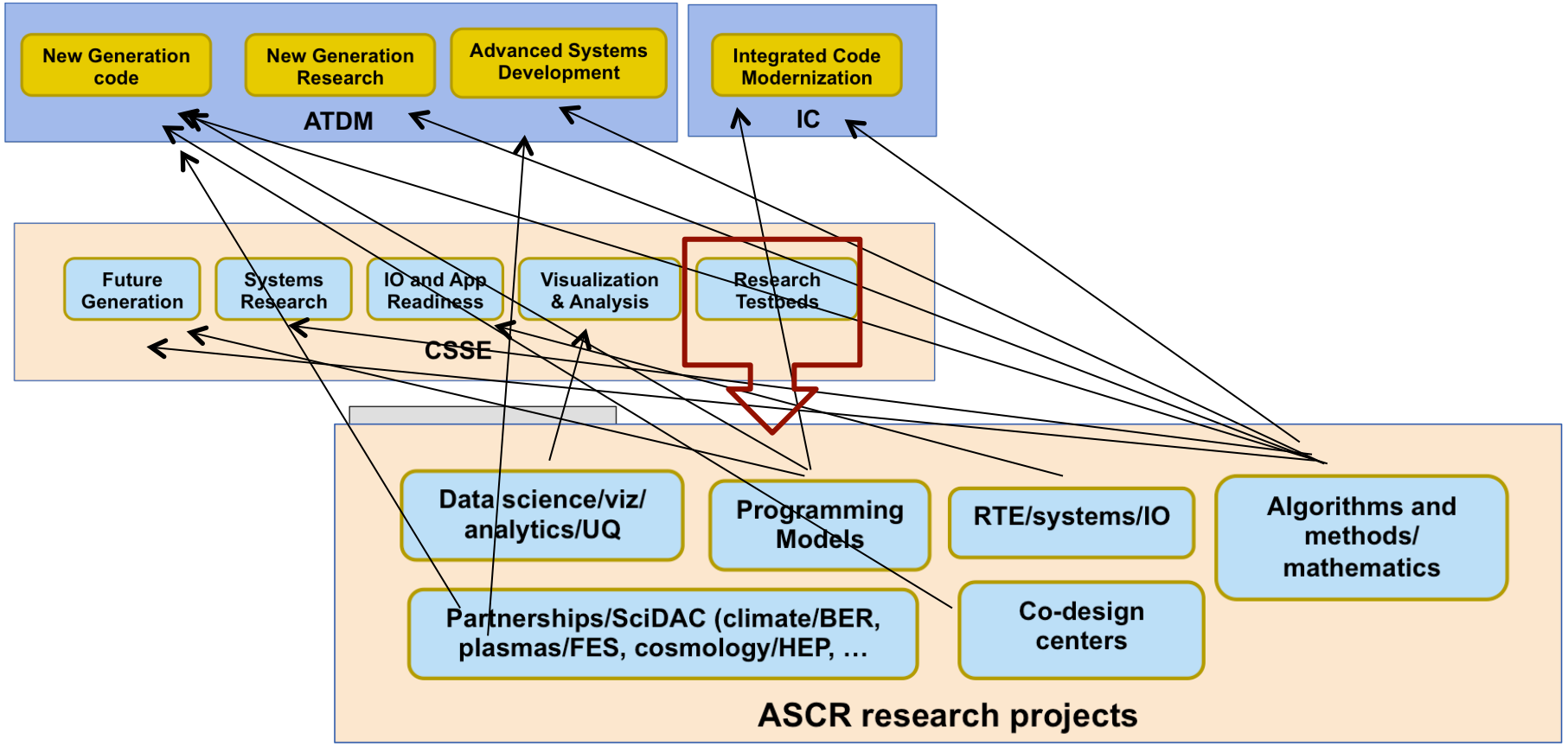


We are exercising our integrated ASCR-enabled approach to co-design across DOE

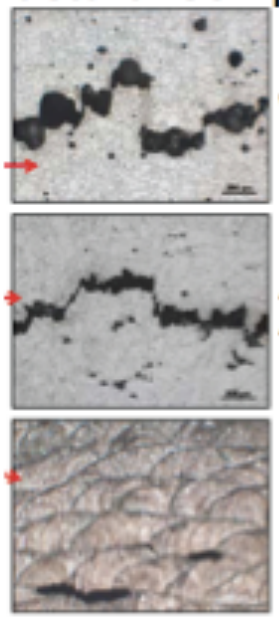
- Stockpile stewardship/ASC
- Office of Science/ASCR
- ASCEM (Advanced Simulation Capability for Environmental Management)
- CCSI (Carbon Capture and Storage Simulation Initiative)
- CASL (Consortium for Advanced Simulation of Light water reactors)
- NRAP (National Risk Assessment Partnership)
- NCI, ECP, ...

Los Alamos has funded projects in every DOE programmatic sector

- **DOE NNSA**
- **DOE SC**
  - ASCR, BES, BER, FES, HEP, NP
  - Many years of solid science research and achievements in all programs
- **DOE Applied Programs**
  - Electricity (grid, m&s, security, …)
  - EERE (renewables, transportation)
  - FE (carbon management, oil and gas)
  - NE (reactors, fuel cycle, innovation)
- **Our programs are well aligned with our national security mission**
- **Many of these involve partnership with other national laboratories and universities**
- **A number of summer schools (co-design, data science at scale, parallel computing)**

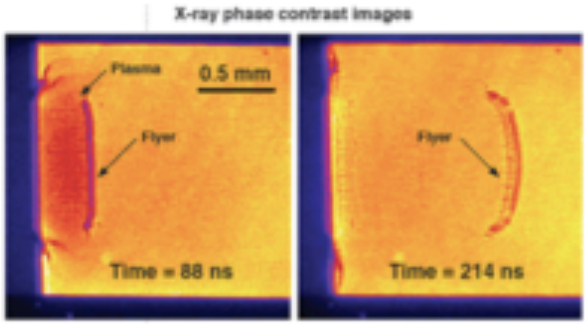
MaRIE will address the control of performance and production of weapons materials at the mesoscale

Performance of additively-manufactured (AM) structural components



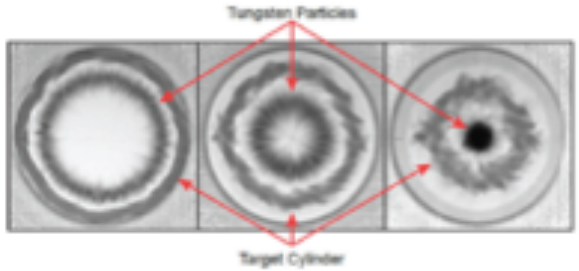
Damage in wrought vs additively-manufactured steel

Detonator performance and safety in LEPs



Movies of exploding bridge wire detonators

Ejecta and Mix in aged components under re-use

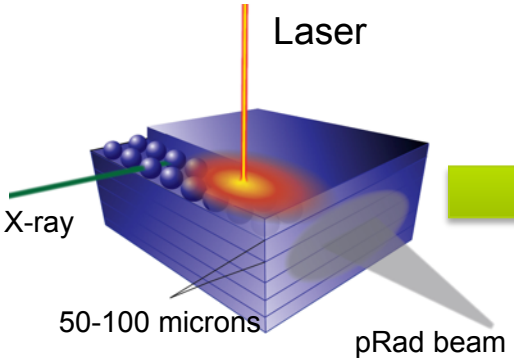


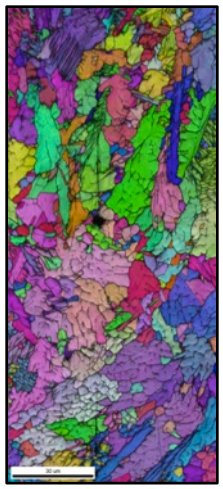
Movies of ejecta in convergent geometry

Requirements for MaRIE are set from analysis of such experiments.
--"(U) MaRIE First Campaigns," LA-CP-15-00501, June, 2015

MaRIE fills a critical gap in length scale between the integral scale addressed by DARHT and U1a and facilities such as NIF and Z.

MaRIE will provide critical data to inform and validate advanced modeling and simulation to accelerate qualification of advanced manufacturing – move from "process-" to "product-based"

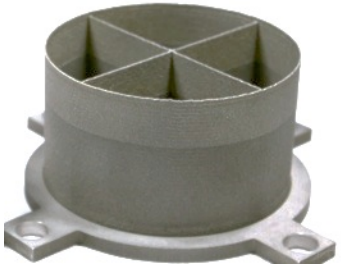


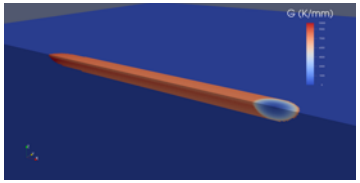


Additively Manufactured 316L Stainless Steel

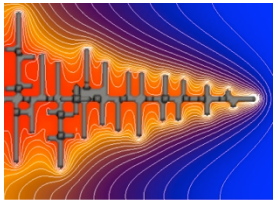
Damage under shock loading unable to coalesce leading to a tougher, more shock resistant material

Prototype Gas Bottle

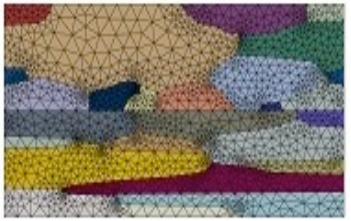




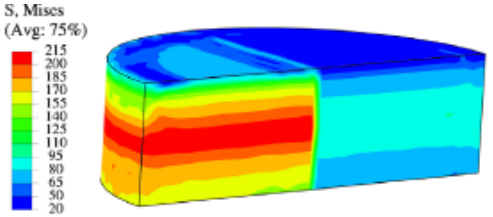
Process Modeling



Microstructure Modeling



Properties Modeling

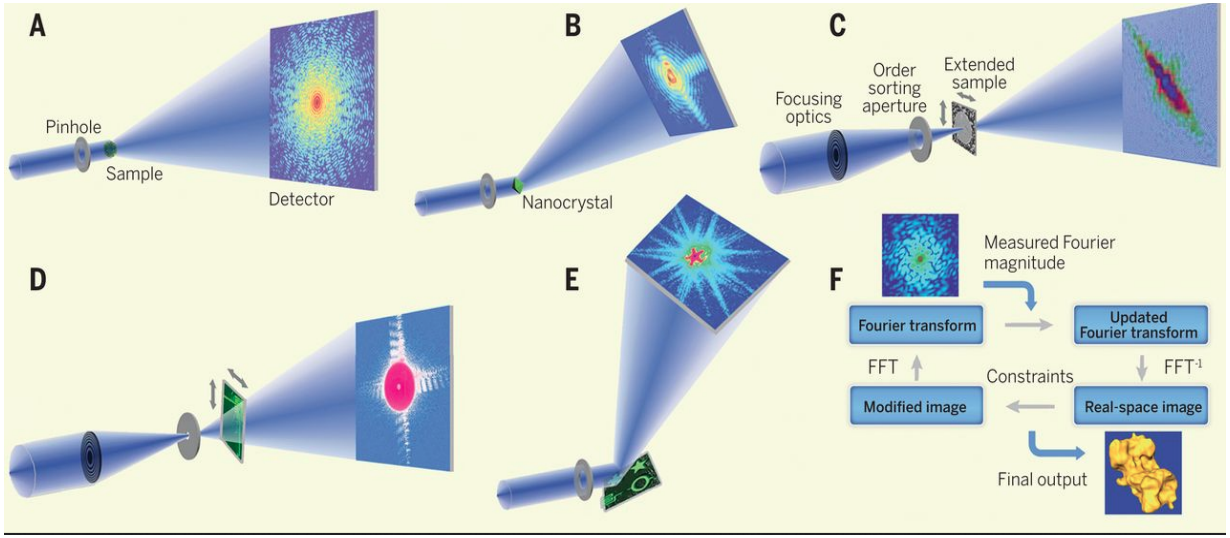


Performance Modeling

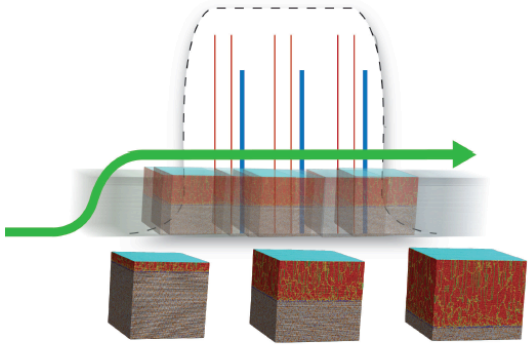
MaRIE and Exascale will enable rapid and confident deployment of new concepts and components through more cost-effective and more rigorous science-based approaches.

To see with time-dependence into and through the mesoscale requires: x-rays; coherent; brilliant and high repetition-rate; of sufficient high energy; and multiple probes at multiple scales

MaRIE builds on the major technical revolutions in: **x-ray lasers** and their brilliance (for time-dependence); and **coherent imaging** (allowing high-resolution observation of non-periodic microstructure).



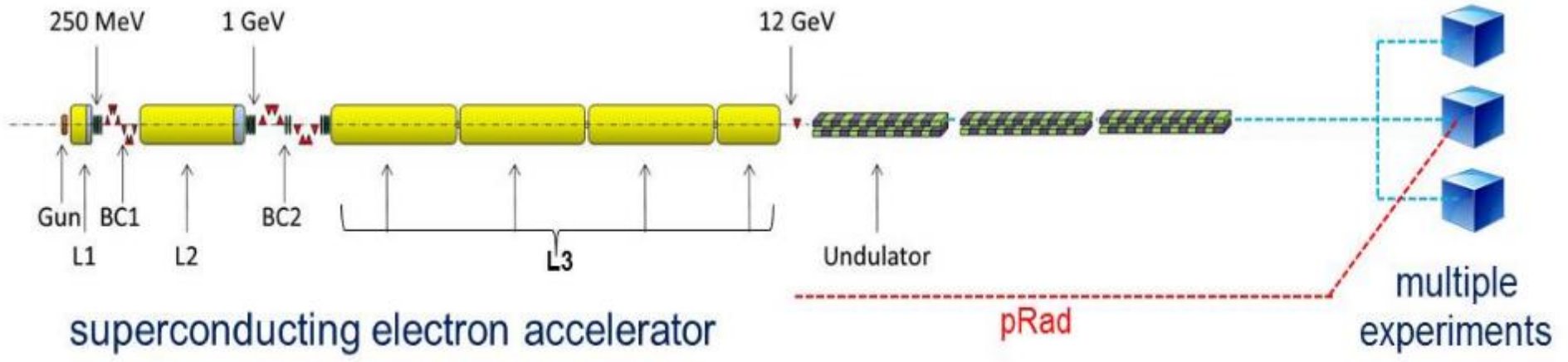
From "Beyond crystallography: Diffractive imaging using coherent x-ray light sources," by J. Miao, T. Ishikawa, I. K. Robinson, and M. M. Murnane, *Science* **348** (1 May 2015), pg 530.



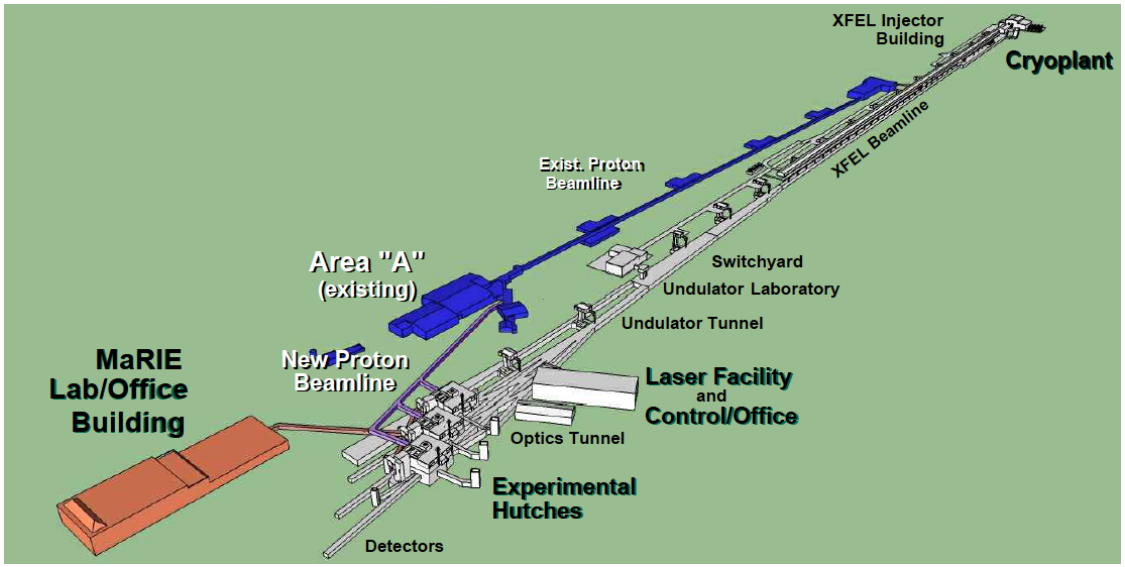
The concept features multiple probes (x rays, protons, electrons, optical photons) to maximize the science.

- **Harder in Energy for mesoscale and high-Z materials**
- **Higher in repetition rate to make movies of microstructure evolution**
- **Multiple probes to support maximum science return**

MaRIE will provide this capability by building a 12-GeV electron linac feeding a 42-keV XFEL with experimental facilities



Our pre-conceptual reference design would be located on the north side of the LANSCE mesa, leveraging the capabilities of that proton/ neutron facility.



Many SC projects are similar to MaRIE 1.0 in scale and complexity and provide benchmarks as well as potential partners

- Basic approach proposed will be to meet essential requirements, then ***maximize*** science capability within TPC and schedule, i.e. "***design to budget***".
- Project will benefit from rigorous SC Project Management Methods including robust Peer Reviews.
- Implementing the SC Process is our proposed risk mitigation approach to lower the risk for MaRIE and meet TPC as the next NNSA Project.


Successful Project Management Practices
in
Office of Science

Daniel R. Lehman, Contractor
L. Edward Temple Jr.
Project Advisor to the Director, ANL

http://science.energy.gov/oaa

February 2015

Topic

Primary Factors for Successful Project Completion

- Clear Ownership, Accountability, and Responsibilities
- Effective Front-End Planning
- Appropriate Project Contingencies
- Sufficient and Stable Funding
- Regular Independent Oversight

Office of Science Peer Reviews

Our goal for computing is …

To be a recognized leader in high performance computing, especially for national security science, at the forefront of computer and computational science

- **Key elements of Laboratory Computing scope**
  - **ASC Computing**
    - Deliver Trinity on the way to Exascale and beyond
    - Provide excellent support to NW mission, including Tri-Lab partnership
  - **SCI Computing**
    - Provide well-stewarded HPC resources to GS community, enabling program growth
  - **Institutional Computing**
    - Focus on institutional computing AND computing at the institution
- **Anticipate, & help define, the frontiers of high performance computing**

LANL has consistently invested internal resources in Institutional Computing

Year	Budget
FY09	$9.3M
FY10	$10.0M
FY11	$10.6M
FY12	$9.3M
FY13	$10.6M
FY14	$13.0M

Institutional Computing (IC) provides high performance computing cycles for open science through a competitive proposal and resource allocation process.

In addition to direct G&A investment, ASC and SC/Climate programs invest in IC in exchange for a dedicated share of available cycles.

HPC division operates ASC and IC infrastructure on behalf of the institution.

Unclassified HPC Systems

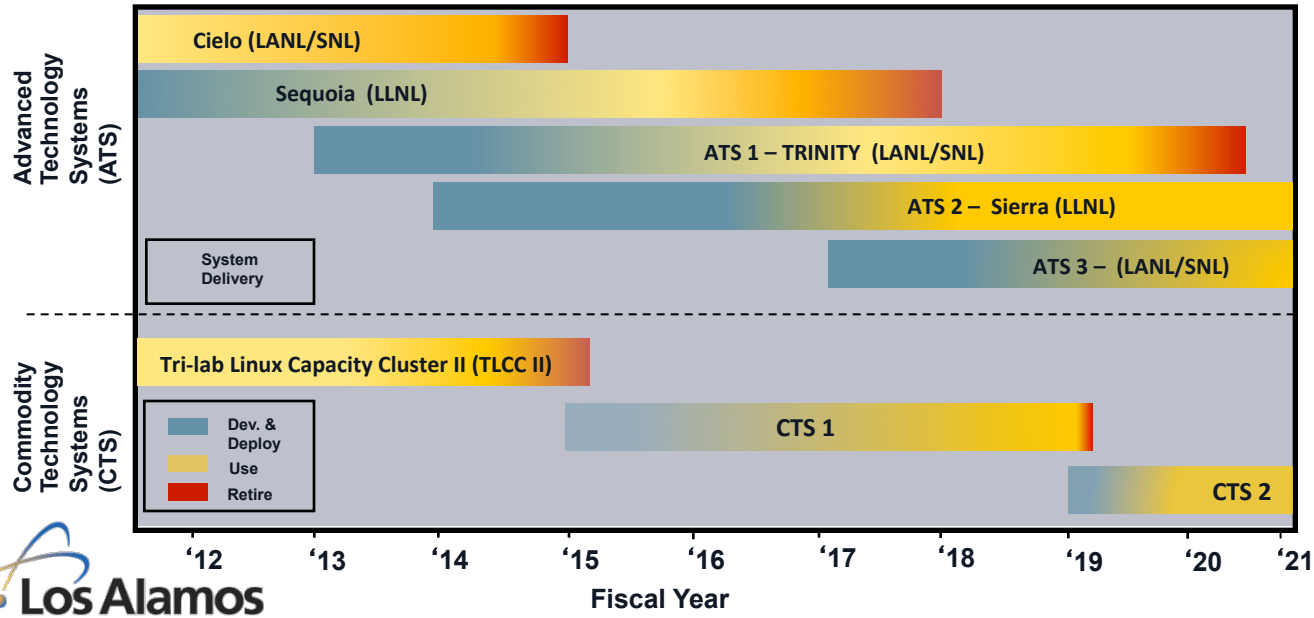
Conejo[1]: SGI, 53 teraflop
Mustang[1]: Appro, 353 teraflop
Pinto[1]: Appro, 51 teraflop
Wolf[1]: Appro, 205 teraflop
Mapache[1]: SGI, 50 teraflop
Moonlight[3]: Appro, 488 teraflop
Cielito[2]: Cray, 10 teraflop
Lightshow: Appro, Visualization

1- Capacity
2- Capability
3- Advanced Architecture

ASC Funded
Institutionally Funded

Trinity, the first Advanced Technology System (ATS) will *enable an increase in Predictive Capability for the NNSA*

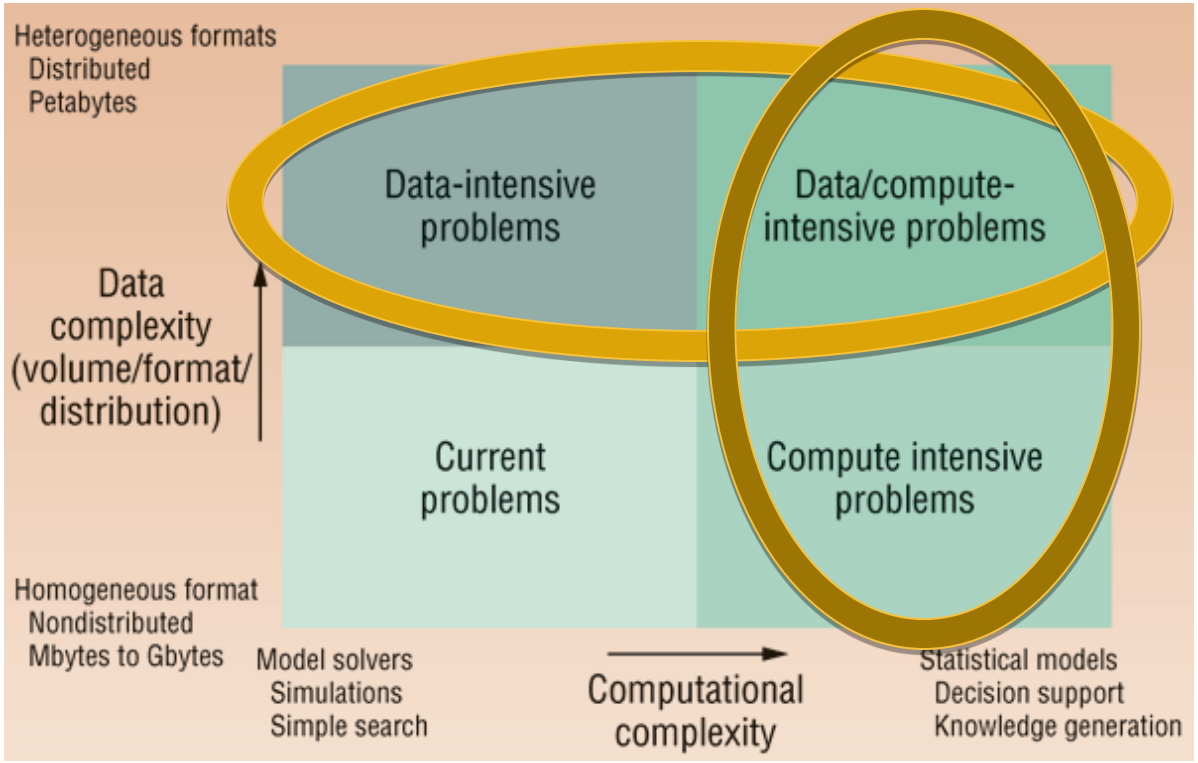
- **Memory capacity is a primary sizing metric (to allow running of large calculations on Trinity)**
- **Trinity needs to demonstrate a significant capability improvement over current platforms (>> Cielo, > Sequoia) in key areas of physics**
  - Improvement is a function of performance (total time to solution), increased geometries and increased physics capabilities
  - Higher fidelity models -> increases in aggregate memory capacity
- **ACES and NERSC are selecting Trinity together**
  - One procurement, two systems
  - Operational consultations on Hopper/Cielo have been useful



New ASC Computing Strategy replaces Capacity/Capability model by Commodity Technology Systems (**CTS**) and Advanced Technology Systems (**ATS**)

LANL is pursuing Data Science along both complexity axes

Ian Gorton, Paul Greenfield, Alex Szalay, Roy Williams, "Data-Intensive Computing in the 21st Century," Computer (4/08)



As with IC & Co-Design, we are investing internal resources in “Big Data:”

-high bandwidth intranet and internet connectivity

-testbed architectures and pilot use-case projects

LANL thoughts on ASCR long range planning elements and priorities

- **The nexus of large data *rates* (MaRIE), large data *sizes* ("LHC"), analytics, machine learning, visualization**
- **Unconventional computing**
- **Novel multi-scale, multi-physics algorithms, methods, and software**
- **Runtime, programming, and too chain research to address data and computational challenges of the future**
- **Co-design: our integrating approach**
  - Experimental design
  - Algorithm and methods design
  - Sensor and computing design
  - Cyber
  - …